

AR201-13955A

RECEIVED
OPPT NCIC

2002 SEP 18 PM 1:55

High Production Volume (HPV) Challenge Program

Data Analysis and Test Plan

For

2,4,7,9-Tetramethyl-5-decyne-4,7-diol

Prepared by:

Air Products and Chemicals, Inc.

7201 Hamilton Boulevard
Allentown, PA 18195

Submitted: December 2001

Revised: July 2002

Table of Contents

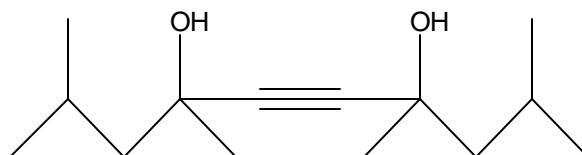
1.0	INTRODUCTION	2
2.0	EVALUATION OF DATA	2
2.1	Physico-chemical Data.....	2
2.1.1	Melting Point	2
2.1.2	Boiling Point.....	2
2.1.3	Vapor Pressure	2
2.1.4	Partition Coefficient	2
2.1.5	Water Solubility	2
2.1.6	Summary of Physico-chemical Data	2
2.2	Environmental Fate and Biodegradation Data.....	2
2.2.1	Photodegradation	2
2.2.2	Hydrolysis	2
2.2.3	Biodegradation.....	2
2.2.4	Transport/Distribution.....	3
2.2.5	Summary of Environmental Fate and Biodegradation Data.....	3
2.3	Ecotoxicology Data	3
2.3.1	Acute Toxicity to Fish.....	3
2.3.2	Acute Toxicity to Aquatic Invertebrates.....	3
2.3.3	Toxicity to Aquatic Plants.....	4
2.3.4	Summary of Ecotoxicology Data	4
2.4	Health Effects Data.....	4
2.4.1	Acute Health Effects	4
2.4.1.1	Acute Oral Toxicity	4
2.4.1.2	Acute Inhalation Toxicity	4
2.4.1.3	Acute Dermal Toxicity	4
2.4.1.4	Summary of the Acute Toxicological Effects	5
2.4.2	Genetic Toxicology Effects.....	5
2.4.2.1	Bacterial Gene Mutation Assay.....	5
2.4.2.2	<i>In Vitro</i> Chromosomal Aberration Assay.....	5
2.4.2.3	Summary of Genetic Toxicology Effects	6
2.4.3	Repeated Dose Health Effects	6
2.4.3.1	Systemic Oral Toxicity	6
2.4.3.2	Reproductive and Developmental Toxicity	6
2.4.3.3	Summary of Systemic, Reproductive and Developmental Toxicity Effects ..	7
3.0	CONCLUSIONS	7
4.0	REFERENCES	9

LIST OF TABLES

Table 1- HPV Data Requirements/Critical Studies for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol.....	8
--	---

1.0 INTRODUCTION

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is an acetylenic diol derived from acetylene and ketone and is used as a surfactant, defoamer, and wetting agent. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has the following structure:



Air Products and Chemicals, Inc. has committed to provide basic chemistry, environmental fate, ecotoxicity and health effects information on 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS 126-86-3) listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. By participating in this voluntary program, Air Products and Chemicals, Inc., agreed to assess the adequacy of existing data; prepare summaries of the data characterizing the chemical; determine data needed to fulfill the HPV data requirements; and design and submit a test plan to satisfy these testing requirements.

2.0 EVALUATION OF DATA

2.1 Physico-chemical Data

- 2.1.1 Melting Point:** 54-55° C (129-131° F) [Ref. 1]
- 2.1.2 Boiling Point:** 262-263° C (504-505° F) [Ref. 2]
- 2.1.3 Vapor Pressure:** 0.66 ± 0.04 Pa @ 20°C ($4.9 \pm 0.3 \times 10^{-3}$ mm Hg) [Ref. 3]
- 2.1.4 Partition Coefficient:** $\log Pow = 2.8$ at 22-22.5°C [Ref. 4]
- 2.1.5 Water Solubility:** 1.70 g/l at 20±0.5°C [Ref. 5]

2.1.6 Summary of Physico-chemical Data

Scientifically reliable data exists for all SIDS physico-chemical endpoints. No additional testing is recommended.

2.2 Environmental Fate and Biodegradation Data

2.2.1 Photodegradation:

Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.05, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.), Atmospheric Oxidation Program (v1.90) modeling component was used to calculate the rate of photodegradation for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The half-life was calculated to be 0.3 days (or 3 hours), assuming the reaction occurred over a 12-hour day with an average atmospheric concentration of 1.5×10^6 OH/cm³ [Ref. 6].

2.2.2 Hydrolysis:

The half-life of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at pHs of 4, 7, and 9 is greater than one year at 25° C (OECD 111). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is hydrolytically stable [Ref. 7].

2.2.3 Biodegradation:

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is not inhibitory towards biomass. In an activated sludge respiratory inhibition test (OECD 209) the 3-hr EC50 was approximately 680 ppm. [Ref. 8] 2,4,7,9-Tetramethyl-5-decyne-4,7-diol degraded approximately 5% in the Modified Sturm test (OECD 301B). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol reached a daily degradation of approximately 25% (last 16 day daily average) in the Semi-Continuous Activated Sludge test (OECD 302A). These tests indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is not readily biodegradable but it is inherently biodegradable [Ref. 9 and 10, respectively].

2.2.4 Transport/Distribution:

The LEV3EPI fugacity model (from EPIWIN V3.05, USEPA) was used for predicting partitioning of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol among air, water, soil and sediment compartments. The following are the concentration results using a soil K_{oc} of 1,670 as calculated by the model and a log K_{ow} of 3.61 as calculated by the KOWWIN (USEPA) program [Ref. 11]:

- Air	0.4%
- Water	29%
- Soil	69%
- Sediment	2%

2.2.5 Summary of Environmental Fate and Biodegradation Data

Scientifically reliable data exists for all SIDS environmental fate and biodegradation endpoints. No additional testing is recommended.

2.3 Ecotoxicology Data

2.3.1 Acute Toxicity to Fish:

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was tested in both fathead minnows and carp according to OECD guideline 203.

Fathead minnows (*Pimephales promelas*) were exposed for 96 hours to concentrations of 0, 4, 8, 16, 32, and 64 mg/l of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in a semi-static system. The 24- and 96-hour LC_{50} values (concentration causing 50% of the fish to die) were determined. All LC_{50} values were the same due to the fact that all deaths occurred within the first 24 hours of the test. The LC_{50} value for 24- and 96-hours was 36 mg/l with 95 percent confidence intervals ranging from 31 to 41 mg/l. [Ref. 12]

Carp (*Cyprinus carpio*) were exposed for 96 hours to concentrations of 0, 10, 18, 32, 56 and 100 mg/l of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in a static system. The 24- and 96-hour LC_{50} values were determined. All deaths occurred within the first 24 hours of the test. The LC_{50} value for 24- and 96- hours was 42 mg/l with 0 percent mortality at 32 mg/l and 100 percent mortality at 56 mg/l. Concentrations down to 18 mg/l induced effects on swimming behavior and pigmentation, while no sub-lethal effects occurred at 10 mg/l. The 96-hour No Observed Effect Level (NOEL) was 10 mg/l. [Ref. 13]

These results indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to fish.

2.3.2 Acute Toxicity to Aquatic Invertebrates:

Daphnia magna were exposed for 24 hours to concentrations of 0, 62.5, 125, 250, 500, and 1000 mg/l. Four groups of 5 daphnia were exposed at each concentration. After 24 hours the number of immobilized Daphnia were counted. The 24-hour EC_{50} value (concentration causing 50% of the daphnia to be immobilized) was determined. The 24-hour EC_{50} was 88 mg/l. The confidence interval could not be calculated due to the lack of partial mortality in at least one concentration. However, this confidence interval would be expected to fall within 62.5 and 125 ppm, which are the chemical concentrations above and below the calculated EC_{50} . [Ref. 14]

Daphnia magna were exposed for 48 hours to concentrations of 0, 18, 32, 45, 100, and 180 mg/l. Two groups of 10 daphnia were exposed at each concentration. After 24 and 48 hours the number of immobilized Daphnia were counted and the 24- and 48-hour EC_{50} values were determined. OECD guideline 202 was followed. The 24-hour EC_{50} for Daphnia magna exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was 99 mg/l based on average exposure concentrations with a 95 percent confidence interval between 83 and 130 mg/l. The 48-hour EC_{50} was 91 mg/l with a 95 percent confidence interval between 81 and 110 mg/l. The 48-hour No Observed Effect Concentration (NOEC) was 43 mg/l. [Ref. 15]

These results indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to aquatic invertebrates.

2.3.3 Toxicity to Aquatic Plants:

Fresh water green algae (*Selenastrum capricornutum*) were examined in a 3-day growth inhibition test. Algal cultures were exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in concentrations ranging from 1 to 100 mg/l, increasing with a factor of 2.2. The mean cell growth and the mean growth rate from each culture were calculated, and the EC₅₀ values (concentration causing 50% reduction in biomass or growth rate) were determined. OECD guideline 201 was followed. The 72-hour EC₅₀ for algal cell growth inhibition (E_BC₅₀) was 15 mg/l with a 95 % confidence interval ranging from 9 to 23 mg/l. The EC₅₀ for algal cell growth rate reduction (E_RC₅₀: 0-72h) was 82 mg/l with a 95 % confidence interval ranging from 39 to 170 mg/l. The NOEC for algal cell growth inhibition and growth rate reduction was 1.0 mg/l. However, a recovery of growth was observed during the last 48 hours of exposure with a NOEC of 4.6 mg/l for growth rate. [Ref. 16]

These results indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to algae.

2.3.4 Summary of Ecotoxicology Data

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to fish, daphnia and algae. Scientifically reliable data exists for all SIDS ecotoxicity endpoints. No additional ecotoxicity testing is recommended.

2.4 Health Effects Data

2.4.1 Acute Health Effects

2.4.1.1 Acute Oral Toxicity

Ten Sprague-Dawley rats were orally administered 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was prepared as a 5% solution in hydrous alcohol. Each rat received a dose volume of 10 ml/kg of body weight. The animals were observed daily post-dose for 14 days. All animals survived, showed no abnormal clinical signs and gained weight. Gross necropsy did not reveal any test material-related pathological changes. The oral LD₅₀ for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rats was greater than 500 mg/kg. [Ref. 17]

2.4.1.2 Acute Inhalation Toxicity

Ten rats were exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol via inhalation. The 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was prepared as a 5% aqueous solution. The test solution was aerosolized to provide a concentration of greater than 20 mg of mist per liter of chamber air over the one-hour period. The test atmosphere was not analyzed. The animals were observed daily for 14 days. All animals survived. Ocular and nasal irritation as well as a reduction in spontaneous activity was noted in all animals immediately following the one-hour exposure. All animals returned to normal within 3 hours. One male and one female were autopsied at random. Gross necropsy did not reveal any test material-related pathological changes. The inhalation LC₅₀ for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rats was greater than 20 mg/l. [Ref. 18]

2.4.1.3 Acute Dermal Toxicity

Six New Zealand White rabbits were exposed dermally to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The neat 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (1,000 mg/kg) was applied to an intact shaved skin site. The entire trunk of each animal was then encased in a plastic sleeve to ensure continuous contact of the test material with the skin for a 24-hour period. The sleeve was removed after 24 hours and the animals were observed daily for 14 days. No dermal erythema or edema was seen in any animal during the 14-day observation period. There was no mortality. The dermal LD₅₀ for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rabbits was greater than 1,000 mg/kg. [Ref. 19]

Five rats of each sex were administered 2,000 mg/kg of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol by dermal application. OECD guideline 402 was followed. No mortality and no clinical signs of ill health were observed during the study. Skin abnormalities on the treated area included scales and

scabs in two females between days 4 and 6. Low body weight gain or body weight loss was noted in all animals over the first week of the study with improved body weight gain over the second week. Macroscopic post mortem examination of the animals at termination did not reveal any significant abnormalities. The dermal LD₅₀ for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rats was greater than 2,000 mg/kg. [Ref. 20]

2.4.1.4 Summary of Acute Toxicological Effects

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is practically non-toxic following a single oral, inhalation, or dermal exposure. Scientifically reliable data exists for all SIDS acute toxicity endpoints. No additional acute toxicity testing is recommended.

2.4.2 Genetic Toxicology Effects

2.4.2.1 Bacterial Gene Mutation Assay

2,4,7,9-Tetramethyl-5-decyne-4,7-diol diluted in dimethylsulfoxide (DMSO) was examined for mutagenic activity in the Salmonella-Escherichia coli/microsome plate incorporation assay. OECD guidelines were followed. The assay was performed using the standard plate incorporation procedure with *S. typhimurium* strains TA1535, TA1537, TA98, and TA100 and *E. coli* strain WP2 (uvrA) over a dose range of 10 to 5,000 ug/plate in both the presence and absence of an Aroclor 1254-induced rat-liver metabolic activation system. The initial experiment used 5 percent (v/v) metabolic activation and the repeat experiment used 10 percent (v/v) metabolic activation. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was not mutagenic under the test conditions used in this bacterial assay. [Ref. 21]

2.4.2.2 In Vitro Chromosomal Aberration Assay

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was tested for its ability to induce chromosome aberrations in Chinese hamster ovary (CHO) cells in the presence and absence of rat S-9 metabolic activation (MA) according to OECD guideline 473.

In the preliminary cytotoxicity assay, CHO cells were exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at concentrations of 19.5, 78.3, 312.5, 1250, and 3500 ug/ml in both the absence and presence of MA. A high dose of 3500 ug/ml was used based on the limit of solubility of the test article in DMSO. Cells were exposed to the test article in the absence of MA for 3 and 21 hours and in the presence of MA for 3 hours. At 21 hours after exposure initiation, cells were harvested and evaluated. All of the cultures from the top two dose levels exhibited a significant decrease in confluency (0 to 25 percent) and therefore were not harvested. For cultures exposed to the test article for 3 hours in the presence or absence of MA, no significant reduction in mitotic index was observed at dose levels of 312.5 ug/ml and below. Cultures exposed for 21 hours to the test article at 312.5 ug/ml showed a significant reduction in mitotic index.

Based on the cytotoxicity results, the initial chromosome aberration study was performed by exposing CHO cells for 3 hours to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at concentrations of 19.5, 39.1, 78.1, 156.3, and 312.5 ug/ml in both the absence and presence of MA. At 21 hours after initiation of exposure, cells were harvested and evaluated. Cytotoxicity was evident in cultures exposed to 312.5 ug/ml both with and without MA, so the cells were not harvested for evaluation. In cultures at the three dose levels scored (39.1, 78.1, and 156.3 ug/ml), there was no statistically significant increase in the number of cells with structural aberrations and the mitotic index was comparable to that for the control. No increases in polyploidy were observed in the presence or absence of MA.

The dose levels for the replicate experiment were based on the results of the cytotoxicity experiment (-MA) and the initial experiment (+MA), which indicated cytotoxicity and a significant reduction in confluency at the 312.5-ug/ml dose level. The replicate experiment was performed by exposing

CHO cells for 21 hours to the test article at concentrations of 9.8, 19.5, 39.1, 78.1, and 156.3 ug/ml in the absence of MA, and for 3 hours at concentrations of 19.5, 39.1, 78.1, and 156.3 ug/ml in the presence of MA. At 21 hours after initiation of exposure, cells were harvested and evaluated. At the three dose levels scored in both MA conditions (39.1, 78.1, and 156.3 ug/ml), there was no statistically significant increase in the number of cells with structural aberrations and the mitotic index was comparable to that for the control. No increases in polyploidy were observed in the presence or absence of MA. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol did not induce structural chromosome damage in this *in vitro* CHO cell system. [Ref. 22]

2.4.2.3 Summary of Genetic Toxicology Effects

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was not mutagenic when examined in an *in vitro* bacterial assay and was not clastogenic when examined in an *in vitro* mammalian cell assay. Scientifically reliable data exists for all SIDS genetic toxicity endpoints. No additional genetic toxicity testing is recommended.

2.4.3 Repeated Dose Health Effects

2.4.3.1 Systemic Oral Toxicity

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was administered in the diet to groups of male and female Long-Evans rats for 28 days. Each group was composed of 6 rats of each sex. The rats were approximately 6-7 weeks of age at the start of the test. The dose levels were 0, 625, 1250, 2500, and 5000 ppm. Test diets were made up on a weekly basis. Statistical analysis of the body weight and food consumption data was performed using the F-test and the Student's t-test. Mortality, physical observations, body weight, and food consumption data, as well as gross necropsy observations did not reveal any adverse effects considered to be attributable to the administration of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at any of the dose levels. The NOEL was 5000 ppm. [Ref. 23]

In a repeated dose oral toxicity study, groups of four male and four female beagle dogs were administered 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in gelatin capsules at dose levels of 0, 200, 250 and 300 mg/kg/day for 91 days. Because the dogs had to be gradually acclimated from 50 mg/kg/day to higher dose levels of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol to avoid vomiting, the total test period was 130 days. The control animals received capsules of granulated table sugar. Capsule administration followed feeding by approximately one hour.

All dogs survived for the duration of this study with few clinical signs. Occasional dogs in the mid- and high-dose groups exhibited sporadic, neurological disturbances (convulsions, tremors) during the study. All other observations, including feed consumption, body weight gains, organ weights (except liver), clinical chemistries, hematology, urinalysis, gross pathology, and histology were judged to reflect no compound-related or biologically significant changes.

This study did not establish a NOEL for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in dogs, since mean liver weights and liver-to-body weight ratios in all treated groups were higher than in the corresponding control groups. However, since no histological abnormalities were observed in these livers, the liver enlargement was judged to be due to hyperplasia of the hepatic endoplasmic reticulum, where xenobiotic/drug metabolizing enzymes are located. [Ref. 24]

2.4.3.2 Reproductive and Developmental Toxicity

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was administered to rats during a single generation reproduction study and for ninety one days to the F1a weanlings. The test material was mixed into the rats' feed to provide dose levels of 0, 500, 1000, and 2000 mg/kg/day.

Sexually mature Sprague-Dawley albino rats were divided into four groups, each consisting of ten male and twenty female rats. Males were sacrificed following the 20th day of breeding and females

were sacrificed when their litters were weaned at 21 days of age. All Fo animals were fed their respective diets from the start of cohabitation until their scheduled sacrifice. The weanlings were randomized to their respective groups and carried on the same dose levels as their parents until the termination of the experiment.

The only pertinent findings observed in the Fo parents were: decreased body weight and feed consumption of the high-dose female group, slight decrease in the mean weaning weight of both male and female pups of the high-dose group, and a slight decrease in the lactation indices of the high-dose group. Histology of the reproductive organs in the Fo parents revealed no abnormalities. Fertility, viability and gestation indices were not affected by treatment.

A slight decrease in the mean rate of body weight gain was observed in the mid- and high-dose F1a male and female rats; there was also a significant decrease in this parameter in the low-dose male group during the first eight weeks. All groups exhibited normal mean hematological, clinical chemistry, and urinalysis findings after 91 days on test. The mid- and high-dose groups exhibited a significant increase in their absolute and relative liver weights. Histopathology of the liver of the mid- and high-dose F1a male and female rats showed mild to moderate centrilobular cloudy swelling of the hepatocytes.

2,4,7,9-Tetramethyl-5-decyne-4,7-diol, when fed to rats under the conditions of this experiment, showed no effect at 500 mg/kg/day but did have a toxic effect in the F1a generation at greater than or equal to 1,000 mg/kg/day while in the reproduction phase of this experiment there was a toxic effect at the 2,000 mg/kg/day level, a borderline effect at the 1,000 mg/kg/day level and no effect at 500 mg/kg/day. [Ref. 25]

2.4.3.3 Summary of Systemic, Reproductive and Developmental Toxicity Effects

Effects on the reproductive organs were assessed in all of the repeated dose studies summarized above. There were no adverse effects on the reproductive organs in males and females examined grossly or histologically at doses up to and including 300 mg/kg in dogs and 2,000 mg/kg in rats.

Repeat-dose studies in rats and dogs showed few effects. A mild effect on the liver was seen in both species.

All of the repeat-dose studies are scientifically reliable. No further testing for systemic, reproductive or developmental effects is recommended.

3.0 CONCLUSIONS

All of the data needed to meet the requirements of the HPV program are available and of high quality. No further studies or data are needed to assess the hazards of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. Table 1 shows the studies that exist for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol.

TABLE 1: HPV DATA REQUIREMENTS/CRITICAL STUDIES: 2,4,7,9-Tetramethyl-5-decyne-4,7-diol

HPV Data Category	Test Endpoint		Acceptable Data Reference (Klimisch Rating)	Data to be Generated
Physical and Chemical Properties	Melting Point		1 (1)	No
	Boiling Point		2 (1)	No
	Vapor Pressure		3 (1)	No
	Partition Coefficient		4 (1)	No
	Water Solubility		5 (1)	No
Environmental Fate and Pathways	Photodegradation		6 (2)	No
	Hydrolysis		7 (1)	No
	Biodegradation		8 (1), 9 (1), 10 (1)	No
	Transport/Distribution		11 (2)	No
Ecotoxicity	Acute toxicity to Fish		12 (2), 13 (1)	No
	Acute toxicity to Aquatic Invertebrates		14 (2), 15 (1)	No
	Toxicity to Aquatic Plants		16 (1)	No
	Chronic aquatic invertebrate test ¹		NR	No
	Terrestrial toxicity ¹		NR	No
Human Health Effects	Acute toxicity		17 (2), 18 (2), 19 (2), 20 (1)	No
	Repeated Dose		23 (2), 24 (2), 25 (2)	No
	Genetic Toxicity	Gene Mutation	21 (1)	No
		Chromosome Aberration	22 (1)	No
	Reproductive Toxicity		25 (2)	No
	Developmental Toxicity		25 (2)	No

Notes:

Data listed are cross-referenced to a Robust Summary report [i.e. 1 (2)]; which identifies the reference number and Klimisch Rating (). If more than one study is listed it means they are co-critical.

¹ = Test are not required for all chemicals; only when appropriate.

NR = Not Required

4.0 REFERENCES

1. Melting Point: Air Products and Chemicals, Inc. (EXT-99/084). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Melting Temperature (OECD 102). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1
2. Boiling Point: Air Products and Chemicals, Inc. (EXT-99/083). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Boiling Temperature (OECD 103). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1
3. Vapor Pressure: Air Products and Chemicals, Inc. (EXT-99/082). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Vapor Pressure (OECD 104). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1
4. Partition Coefficient: Air Products and Chemicals, Inc. (EXT-99/100). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Partition Coefficient (N-Octanol/Water) (OECD 117). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1
5. Water Solubility: Air Products and Chemicals, Inc. (EXT-99/099). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Water Solubility (OECD 105). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1
6. Photodegradation: Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.05, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.) Atmospheric Oxidation Program (v1.90). Klimisch = 2
7. Hydrolysis: Air Products and Chemicals, Inc. (EXT-00/001). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Hydrolysis as a Function of pH (OECD 111). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1
8. Biodegradation: Air Products and Chemicals, Inc. (PFT-99/004). Activated Sludge, Respiration Inhibition Testing, OECD 209 for Surfynol 104 Surfactant. Testing Facility: SGS U.S. Testing Company Inc., Fairfield, New Jersey, USA. Study year: 1999. Klimisch = 1
9. Biodegradation: Air Products and Chemicals, Inc. (EXT-99/097). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of "Ready" Biodegradability: Carbon Dioxide (CO₂) Evolution Test (Modified Sturm Test) (OECD 301B). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1
10. Biodegradation: Air Products and Chemicals, Inc. (PFT-99/004). Semi-Continuous Activated Sludge Test (OECD Method 302A) for Surfynol 104 Surfactant. Testing Facility: SGS U.S. Testing Company Inc., Fairfield, New Jersey, USA. Study year: 1999. Klimisch = 1
11. Transport/Distribution: Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.05, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.) LEV3EPI Fugacity Model. Klimisch = 2
12. Acute Toxicity to Fish: Air Products and Chemicals, Inc. (EXT-92/040). Surfynol 104 Fish Toxicity Results. Testing Facility: Commonwealth Technology, Inc., Lexington, Kentucky, USA. Study year: 1991. Klimisch = 2
13. Acute Toxicity to Fish: Air Products and Chemicals, Inc. (EXT-00/007). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (Static): 96-Hour Acute Toxicity Study In Carp (OECD 203). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1

14. Acute Toxicity to Aquatic Invertebrates: Air Products and Chemicals, Inc. (EXT-92/040). Surfynol 104 Fish Toxicity Results. Testing Facility: Commonwealth Technology, Inc., Lexington, Kentucky, USA. Study year: 1991. Klimisch = 2
15. Acute Toxicity to Aquatic Invertebrates: Air Products and Chemicals, Inc. (EXT-99/101). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Static Toxicity Study In Daphnia Magna (OECD 202, Part 1). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1
16. Toxicity to Aquatic Plants: Air Products and Chemicals, Inc. (EXT-00/030). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Fresh Water Algal Growth Inhibition Test (OECD 201). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1
17. Acute Oral Toxicity: Air Products and Chemicals, Inc. (EXT-86/020). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Toxicity Studies. Testing Facility: Foster D. Snell Biological Sciences Laboratory, Elizabeth, New Jersey, USA. Study year: 1971. Klimisch = 2
18. Acute Inhalation Toxicity: Air Products and Chemicals, Inc. (EXT-86/020). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Toxicity Studies. Testing Facility: Foster D. Snell Biological Sciences Laboratory, Elizabeth, New Jersey, USA. Study year: 1971. Klimisch = 2
19. Acute Dermal Toxicity: Air Products and Chemicals, Inc. (EXT-86/020). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Toxicity Studies. Testing Facility: Foster D. Snell Biological Sciences Laboratory, Elizabeth, New Jersey, USA. Study year: 1971. Klimisch = 2
20. Acute Dermal Toxicity: Air Products and Chemicals, Inc. (EXT-94/012). Assessment of Acute Dermal Toxicity with Surfynol 104 in the Rat. Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1993. Klimisch = 1
21. Gene Mutation: Air Products and Chemicals, Inc. (EXT-99/078). Evaluation of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in the Salmonella-Escherichia Coli/Microsome Plate Incorporation Assay (OECD 471). Testing Facility: SRI International Toxicology Laboratory, Menlo Park, California, USA. Study year: 1999. Klimisch = 1
22. Chromosome Aberration: Air Products and Chemicals, Inc. (EXT-99/091). Evaluation of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in the CHO Chromosome Aberration Assay (OECD 473). Testing Facility: SRI International Toxicology Laboratory, Menlo Park, California, USA. Study year: 1999. Klimisch = 1
23. Systemic Oral Toxicity: Air Products and Chemicals, Inc. (EXT-77/016). A Four-Week Dose Range-Finding Study of Surfynol-104 In Rats. Testing Facility: Bio/dynamics Inc., East Millstone, New Jersey, USA. Study year: 1977. Klimisch = 2
24. Systemic Oral Toxicity: Air Products and Chemicals, Inc. (EXT-94/090). Surfynol 104 - Modified 91-Day Feeding Study In The Dog. Testing Facility: Pharmacopathics Research Laboratories, Laurel, Maryland, USA. Study year: 1979. Klimisch = 2
25. Reproductive and Developmental Toxicity: Air Products and Chemicals, Inc. (EXT-97/005). Surfynol 104: I. Single Generation Reproduction Study in the Rat (Fo-F1a). II. 91-Day Feeding Study (F1a Rats). Testing Facility: Pharmacopathics Research Laboratories, Laurel, Maryland, USA. Study year: 1979. Klimisch = 2